Usable assembly language for GPUs

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319 ms: rpes/src/cuda
183 ms: rpes/src/qhasm (new)

Measured on behemoth:
1.30GHz GTX 280 × 2;
2.83GHz Core 2 Quad Q9550
1974 Knuth:
“There is no doubt that the ‘grail’ of efficiency leads to abuse. Programmers waste enormous amounts of time thinking about, or worrying about, the speed of noncritical parts of their programs, and these attempts at efficiency actually have a strong negative impact when debugging and maintenance are considered. We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil.”
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You’ve tried many algorithms. Tried many software rewrites. Computer is still too slow. Now what?
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Advantage of this answer: full control over CPU! Programmer can control details of memory layout, instruction selection, instruction scheduling, etc.

Compiler can be quite stupid: often fails to exploit CPU, even with programmer’s help.
Yet another answer: Move critical lines to a GPU.

Most common GPU architectures: Evergreen, Northern Islands from AMD; Tesla, Fermi from NVIDIA. In this talk I’ll focus on the Tesla GPU architecture. Tesla GPUs are very easy to find: GTX 280; GTX 295; AC; Lincoln; Longhorn; etc.
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Advantage of this answer: GPU can do huge number of floating-point operations/second.
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Move critical lines to a GPU and write them in asm? This is easier said than done.
2010 L.-S. Chien “Hand-tuned SGEMM on GT200 GPU”:
Successfully gained speed using van der Laan’s decuda, cudasm and manually rewriting a small section of ptxas output.

But this was “tedious” and hampered by cudasm bugs: “we must extract minimum region of binary code needed to be modified and keep remaining binary code unchanged . . . it is not a good idea to write whole assembly manually and rely on cudasm.”
2010 Bernstein–Chen–Cheng–Lange–Niederhagen–Schwabe–Yang “ECC2K-130 on NVIDIA GPUs”; focusing on GTX 295:

Extensive optimizations in CUDA for “ECC2K-130” computation: 26 million iterations/second.

Built new assembly language qhasm–cudasm for Tesla GPUs. Built 90000-instruction kernel entirely in assembly language; later reduced below 10000. 63 million iterations/second for the same computation.
My talk today: Another qhasm-cudasm case study.

2010.11 email from Kindratenko: rpes kernel in particular is of a very much interest to us because it is similar to some of the kernels Alex has implemented. ... We would be very much interested in understanding how this kernel can be re-implemented in the nvidia gpu assembly language that you have developed and what benefits this would give us.
1953 Tom Lehrer “Lobachevsky”:

“I am never forget the day I am given first original paper to write. It was on analytic and algebraic topology of locally Euclidean parameterization of infinitely differentiable Riemannian manifold. Bozhe moi! This I know from nothing. What I am going to do.”
Download rpes in parboil1. Find three implementations of the same computation: base, cuda_base, cuda. Note: no rpes in parboil2; and TeraChem source isn’t public.

./parboil run rpes cuda default -S: 319 milliseconds
= 147 ms on one GPU
+ 94 ms on one CPU core
+ 78 ms copying data.

cuda_base: slower.
base: 63075 ms; no GPU.
Read code to understand it. base has only 600 lines.

CalcOnHost in base: 46-line main computation inside eight nested loops.

Main computation loads data, does some arithmetic, calls a few simple subroutines: e.g., H_dist2 computes $(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2$.

Also one complicated subroutine, root1f, 75 lines, computing $\text{erf}(\sqrt{x})/\sqrt{4x/\pi}$ given $x$. 
Sample input used by parboil:

$x, y, z$ coordinates for 30 atoms:
20 H atoms and 10 O atoms.

Each O atom has 17 “primitives” ($\alpha, c$) organized into 3 shells.
Same primitives, shells for each O:
3rd shell is always $(0.3023, 1)$;
2nd shell is 8 primitives starting $(11720, -0.000314443412)$; etc.

H atom: 4 primitives in 2 shells.

Overall input data:
250 vectors $(x, y, z, \alpha, c)$
organized into 70 shells.
Have $250^4 = 3906250000$ ways to choose four vectors 

$v_1 = (x_1, y_1, z_1, \alpha_1, c_1),$

$v_2 = (x_2, y_2, z_2, \alpha_2, c_2),$

$v_3 = (x_3, y_3, z_3, \alpha_3, c_3),$

$v_4 = (x_4, y_4, z_4, \alpha_4, c_4)$

out of this input.

46-line main computation uses $< 100$ floating-point ops to compute an “integral” $P(v_1, v_2, v_3, v_4)$ given a choice of four vectors.
$70^4 = 24010000$ choices of $w_1 = (x_1, y_1, z_1, \text{shell}_1)$,
$w_2 = (x_2, y_2, z_2, \text{shell}_2)$,
$w_3 = (x_3, y_3, z_3, \text{shell}_3)$,
$w_4 = (x_4, y_4, z_4, \text{shell}_4)$.

Define $S(w_1, w_2, w_3, w_4)$ as $\sum P(v_1, v_2, v_3, v_4)$.

Output of computation:
$70^4$ floats $S(w_1, w_2, w_3, w_4)$.

Actually, \texttt{rpes} computes only
$70 \cdot 71 \cdot 72 \cdot 73/24 = 1088430$ floats from $187240905$ integrals:
apparently there’s a symmetry between $w_1, w_2, w_3, w_4$. 
GPU has 240 32-bit ALUs (arithmetic-logic units; mislabelled “cores” by NVIDIA). Each ALU: one op per cycle; 1.3 \cdot 10^9 cycles per second.

In cuda’s 319 ms: GPU can do 10.0 \cdot 10^{10} ops, as complicated as multiply-add. In 146 ms: 4.3 \cdot 10^{10} ops.

GPU is actually computing 187240905 integrals, each < 100 ops: total < 1.9 \cdot 10^{10} ops. ALUs are sitting mostly idle!
So I wrote a new rpes using qhasm-cudasm.

Integrated into parboil1, put online for you to try:

```
wget http://cr.yp.to/qhasm/parboilrpes.tar.gz

tar -xzf parboilrpes.tar.gz

cd parboilrpes

(x='pwd'; cd common/src;
 make PARBOIL_ROOT=$x)

./parboil run rpes cuda
default -S

./parboil run rpes qhasm
default
Typical code in cudasm:

```assembly
add.rn.f32 $r1, $r20, -$r21
mul.rn.f32 $r6, $r1, $r1
add.rn.f32 $r1, $r24, -$r25
mad.rn.f32 $r6, $r1, $r1, $r6
add.rn.f32 $r1, $r28, -$r29
mad.rn.f32 $r6, $r1, $r1, $r6
```

These instructions work without any of our cudasm bug fixes.
Same code in C/C++/CUDA:

\[
\begin{align*}
dx_{12} &= x_1 - x_2; \\
dy_{12} &= y_1 - y_2; \\
dz_{12} &= z_1 - z_2; \\
dist_{12} &= dx_{12} \times dx_{12} \\
            &\quad + dy_{12} \times dy_{12} + dz_{12} \times dz_{12};
\end{align*}
\]

Compiler selects instructions (e.g., mad for \(*+\)); schedules instructions; assigns registers.
Same in qhasm-cudasm:

dx12 = approx x1 - x2
dy12 = approx y1 - y2
dz12 = approx z1 - z2
dist12 = approx dx12 * dx12
approx dist12 += dy12 * dy12
approx dist12 += dz12 * dz12

Each line is an instruction. Programmer can assign
some or all registers, but qhasm includes a
state-of-the-art allocator.
CUDA:

\[ w = 31.00627668 \times \text{rsqrtf}(X); \]

qhasm-cudasm:

\[ w = \text{approx} \frac{1}{\sqrt{X}} \]

\[ w = \text{approx} \ w \times 31.00627668 \]

cudasm:

\[ \text{rsqrt.f32} \quad \$r7, \; \$r7 \]

\[ \text{mul.rn.f32} \quad \$r7, \; \$r7, \; 0x41f80cdb \]
Start 7680 threads on GPU: 30 blocks of 256 threads; i.e., 256 threads on each core.

Split the 1088430 outputs across these threads: thread $t$ computes outputs $t, t + 7680, t + 15360$, etc.
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Oops, imbalance: slowest thread computes 50341 integrals; average computes \( < 25000 \). GPU is 50% idle!
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Easy fix, not implemented yet: sort shells by # primitives. Reduces penalty to $\approx 10\%$. 
Each GPU core has SRAM:
16384 32-bit registers
split between threads;
16384 bytes “shared memory”
accessible by all threads.

CPU copies atom data from
CPU DRAM to GPU DRAM.
GPU DRAM is very slow,
so threads begin by copying
atom data to shared memory.
Threads also initialize shared
erfseries[X][i] as
\[\sum_j (-1)^j \binom{j}{i} (X/16)^{j-i}/j!(2j + 1)\]
so that
\[(\sqrt{\pi}/2) \text{erf}\sqrt{x + \epsilon}/\sqrt{x + \epsilon} = \sum_i \text{erfseries}[16x][i] \epsilon^i.\]
(Tweak: \(2\pi^{2.5}\) scaling.)
\(i \leq 7\) is adequate
for full float precision.
Maybe even overkill
for the application.